

# The Quantum Liouville Equation is non-Liouvillian

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(Dated: October 17, 2014)

The Hamiltonian flow of a classical, time-independent, conservative system is incompressible, it is Liouvillian. The analog of Hamilton's equations of motion for a quantum-mechanical system is the quantum-Liouville equation. It is shown that its associated quantum flow in phase space, Wigner flow, is not incompressible. It gives rise to a quantum analog of classical Hamiltonian vector fields: the Wigner phase space velocity field  $\mathbf{w}$ , the divergence of which can be unbounded. The loci of such unbounded divergence form lines in phase space which coincide with the lines of zero of the Wigner function. Along these lines exist characteristic pinch points which coincide with stagnation points of the Wigner flow.

PACS numbers: 03.65.-w, 03.65.Ta

## I. INTRODUCTION

In classical phase space the coordinates  $\mathbf{r} = (\mathbf{q}, \mathbf{p})$  are position  $\mathbf{q}$  and momentum  $\mathbf{p}$  with the associated dynamics described by the Hamiltonian velocity field  $\mathbf{v} = (\dot{\mathbf{q}}, \dot{\mathbf{p}})$  giving rise to a continuity equation  $\frac{\partial}{\partial t}\rho(\mathbf{r};t) + \nabla \bullet \mathbf{j}(\mathbf{r};t) = \sigma(\mathbf{r};t)$  for the movement of the classical probability density  $\rho$  and its flow  $\mathbf{j}$ . Because probability is locally conserved the source term  $\sigma(\mathbf{r};t) = 0$ .

Famously, classical Hamiltonian vector fields for time-independent conservative systems are

$$\text{divergence-free} \quad \nabla \bullet \mathbf{v} = 0, \quad (1)$$

$$\text{or, the flow is incompressible} \quad \frac{D\rho}{Dt} = 0. \quad (2)$$

Eq. (2) follows from (1) if the density is made up of ‘‘carriers’’, particles or charges (and their respective probability distributions), such that the flow  $\mathbf{j}$  can be decomposed into the product

$$\mathbf{j} = \rho \mathbf{v}. \quad (3)$$

Then, the *total derivative* [1] of  $\rho$  is  $\frac{D\rho}{Dt} = -\rho \nabla \bullet \mathbf{v}$ .

In quantum mechanics, Wigner's quantum phase space-based distribution function  $W$  [2, 3] obeys [2] the, so-called, quantum Liouville equation [4]

$$\frac{\partial W(\mathbf{r};t)}{\partial t} + \nabla \bullet \mathbf{J}(\mathbf{r};t) = 0, \quad (4)$$

where  $\mathbf{J}$  is the Wigner flow [5] of the system.

Here we establish that the quantum Liouville equation is typically non-Liouvillian, that Wigner's phase space velocity  $\mathbf{w}$ , the quantum analog of  $\mathbf{v}$ , can have unbounded divergence, and that the structure of the divergence of  $\mathbf{w}$  can help us to investigate the phase space structure of a quantum system's dynamics.

We first review features of Wigner flow and introduce the concept of the Wigner phase space velocity  $\mathbf{w}$  (10), in

section II. We then consider quantum systems for which the flow of  $\mathbf{w}$  is always incompressible (harmonic oscillator), in section III, incompressible for energy eigenstates only (‘squared’ harmonic oscillator), in section IV, and generically non-Liouvillian (anharmonic oscillator), in section V, before we conclude in section VI.

## II. WIGNER FLOW

From now on, we will only consider motion in one spatial dimension  $x$ . In this case  $W$  is a one-dimensional Fourier transform

$$W_\varrho(x, p; t) \equiv \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dy \varrho(x+y, x-y, t) \cdot e^{\frac{2i}{\hbar}py}, \quad (5)$$

of the off-diagonal coherences  $\varrho(x+y, x-y, t)$  of the quantum mechanical density matrix  $\varrho$  which has the form  $\varrho = \Psi^*(x+y, t)\Psi(x-y, t)$  if the system is in a pure state  $\Psi$  (star ‘\*’ denotes complex conjugation);  $\hbar = h/(2\pi)$  is Planck's constant rescaled.

$W$  is real valued but can be negative [2] and therefore is a quantum-mechanical ‘quasi-probability’ function [3, 4].

For time-independent conservative systems such as a point mass  $M$  moving under the influence of a potential  $U$ , described by the Hamiltonian

$$H(x, p) = \frac{p^2}{2M} + U(x), \quad (6)$$

where the potential  $U(x)$  can be Taylor-expanded (giving rise to finite forces only),  $\mathbf{J}$  of (4) has the explicit form [2]

$$\mathbf{J} = \begin{pmatrix} J_x \\ J_p \end{pmatrix} = \begin{pmatrix} \frac{p}{M} W \\ - \sum_{l=0}^{\infty} \frac{(i\hbar/2)^{2l}}{(2l+1)!} \partial_p^{2l} W \partial_x^{2l+1} U \end{pmatrix}. \quad (7)$$

Here, the notation  $\partial_x^l = \frac{\partial^l}{\partial x^l}$ , etc., is used for conciseness. Explicit reference to dependence on  $\mathbf{r}$  and  $t$  is now dropped.

Wigner flow's complicated form makes it non-trivial to work out its overall structure.

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To characterize Wigner flow it is useful to determine its orientation winding number [5] (or Poincaré index)

$$\omega(\mathcal{L}, t) = \frac{1}{2\pi} \oint_{\mathcal{L}} d\varphi. \quad (8)$$

The Poincaré index  $\omega$  tracks the orientation angle  $\varphi$  of the flow vectors  $\mathbf{J}$  along continuous, closed, self-avoiding loops  $\mathcal{L}$  in phase space. Because the components of the flow are continuous functions,  $\omega$  is zero except for the case when the loop contains stagnation points. In such a case a non-zero value of  $\omega$  can occur and this value is conserved unless the system's dynamics transports a stagnation point across  $\mathcal{L}$  [5].

When comparing Wigner flow with classical Hamiltonian flow, it is not unreasonable to argue that the first order terms of Wigner flow (7) have classical form

$$\begin{pmatrix} J_x \\ J_p \end{pmatrix} = \begin{pmatrix} v_x W \\ -W \partial_x V \end{pmatrix} + \begin{pmatrix} 0 \\ \mathcal{O}(\hbar^2) \end{pmatrix}; \quad (9)$$

and therefore, whenever higher order quantum terms  $\mathcal{O}(\hbar^2)$  are present, Wigner flow cannot be Liouvillian [6]. It turns out that for eigenstates of Kerr oscillators (section IV, below) this is not correct though.

We note that, firstly, Wigner's function typically has areas of negative value which is why classical probability arguments have to be used cautiously. Secondly, a clear identification of the terms responsible for deviation from the classical case might be of interest in its own right. And, thirdly, we have, so far, little intuition regarding the behaviour of Wigner flow, and we show here that the divergence of its flow can be tied to other physical phenomena, such as the formation of stagnation points of  $\mathbf{J}$  in phase space.

To establish that in general quantum phase space flow is non-Liouvillian, let us cast it into a form analogous to Eq. (3), namely  $\mathbf{J} = W\mathbf{w}$ , and investigate the divergence of the *Wigner phase space velocity*

$$\mathbf{w} = \frac{\mathbf{J}}{W}. \quad (10)$$

According to Eq. (1), to establish when Wigner flow is Liouvillian, we determine when

$$\nabla \bullet \mathbf{w} = 0. \quad (11)$$

With  $\nabla \bullet \mathbf{J} = W \nabla \bullet \mathbf{w} + \mathbf{w} \bullet \nabla W = -\partial_t W$  we have

$$\nabla \bullet \mathbf{w} = -\frac{\mathbf{J} \bullet \nabla W + W \partial_t W}{W^2}. \quad (12)$$

### III. WIGNER FLOW OF HARMONIC OSCILLATORS

For a harmonic potential  $U^\circ(x) = \frac{k}{2}x^2$  with spring constant  $k$ , Wigner flow (7) has the ‘classical’ form

$$\mathbf{J}^\circ = \begin{pmatrix} J_x^\circ \\ J_p^\circ \end{pmatrix} = W^\circ(x, p, t) \cdot \begin{pmatrix} \frac{p}{M} \\ -kx \end{pmatrix}. \quad (13)$$

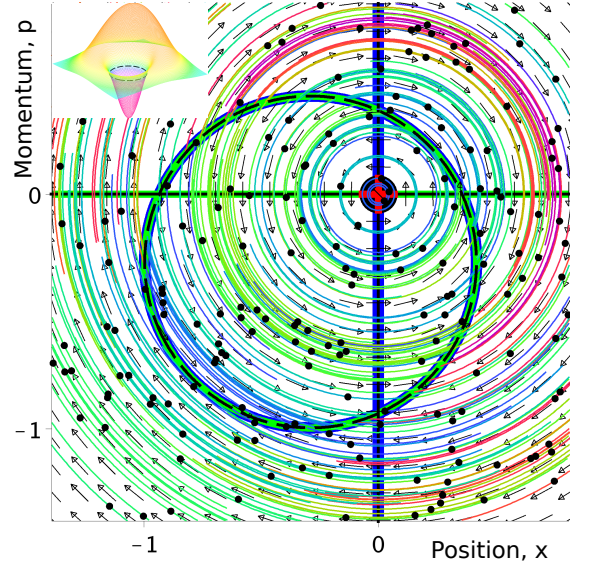


FIG. 1. (Color online) Normalized Wigner flow  $\mathbf{J}/|\mathbf{J}|$  with its streamlines for superposition state  $\Psi = \cos(\frac{\pi}{3})|0\rangle + \sin(\frac{\pi}{3})e^{-i\frac{7}{4}\pi}|1\rangle$  of a harmonic oscillator; with  $M = 1$ ,  $k = 1$  and  $\hbar = 1$ . The streamlines, which were randomly picked and coloured, are *circular*. Despite quantum mechanical flow inversion [5] for  $W < 0$  (see inset), the harmonic oscillator's Wigner flow is always Liouvillian. The black dashed line on top of the green circle depicts the line of zero of the Wigner function (see inset). The red cross at the origin marks the position of the flow's stagnation point, around the potential minimum, with Poincaré index  $\omega = 1$ .

Inserting (13) into (12) yields  $\nabla \bullet \mathbf{w}^\circ = 0$ , always. A harmonic oscillator's quantum phase space flow is always Liouvillian, see Fig. 1.

### IV. WIGNER FLOW OF THE KERR OSCILLATOR

An example of a system for which its energy eigenstates yield Liouvillian Wigner flow, but its superposition states do not, is the ‘squared’ harmonic oscillator, described by the Kerr Hamiltonian

$$\hat{\mathcal{H}}_K = \left( \frac{\hat{p}^2}{2M} + \frac{k}{2}\hat{x}^2 \right) + \Lambda^2 \left( \frac{\hat{p}^2}{2M} + \frac{k}{2}\hat{x}^2 \right)^2. \quad (14)$$

The parameter  $\Lambda$  parameterizes the system's (quantum-optical) Kerr-non-linearity,  $\Lambda \propto \sqrt{\chi^{(3)}}$  [7–10], i.e. in field operator language  $\hat{\mathcal{H}}_K = (a^\dagger a + \frac{1}{2})^2 + \tilde{\chi}^{(3)} (a^\dagger a + \frac{1}{2})^2$ . The wavefunctions of the harmonic oscillator are solutions to the Kerr Hamiltonian rendering the entire system analytically solvable.

Note that  $\hat{\mathcal{H}}_K$  contains products in  $\hat{x}$  and  $\hat{p}$ , this implies that the terms for the Wigner flow are not of the form (7). Instead, the Wigner flow components can be determined using Moyal brackets [6] and are found to be of the form [11]

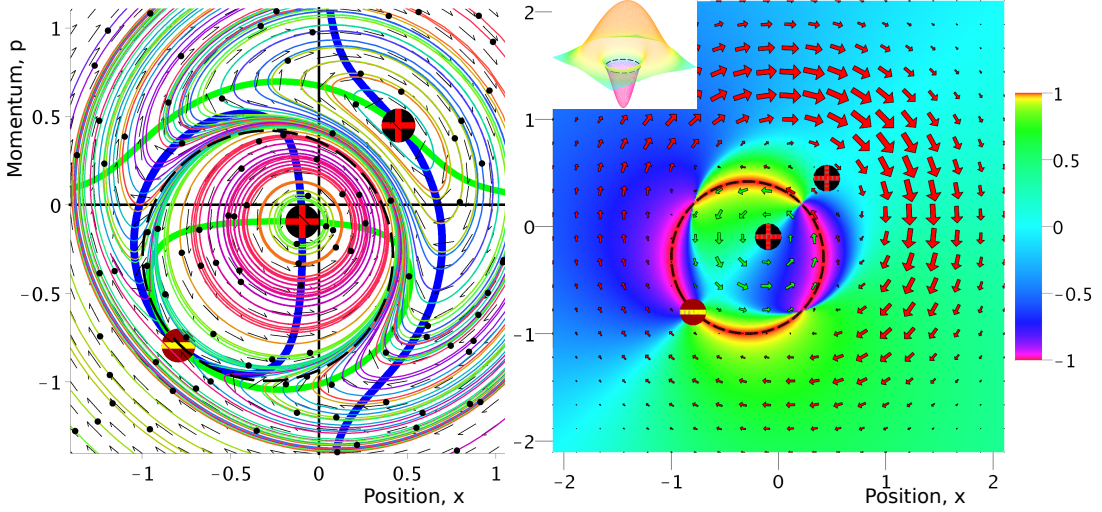


FIG. 2. (Color online) Behaviour of superposition state  $\Psi$  for the Kerr oscillator (14) with  $\Lambda = 2$ , all other parameters as in Fig. 1. Left: Streamlines of Wigner flow  $\mathbf{J}$  and its stagnation points. Yellow minus signs mark stagnation points with Poincaré index  $\omega = -1$ . Right:  $\frac{2}{\pi} \arctan(\nabla \bullet \mathbf{w})$  with Wigner flow  $\mathbf{J}$  superimposed.  $\nabla \bullet \mathbf{w} \neq 0$  almost everywhere: for superposition states quantum phase space flow of the Kerr system is non-Liouvillian. The black dashed line marks the zero of the Wigner function (see inset), at its location, according to Eq. (12), the divergence of  $\mathbf{w}$  becomes unbounded (see right panel).

$$J_x = \left[ \Lambda^2 \left( -\frac{\hbar^2 p}{4M^2} \partial_x^2 + \left\{ \frac{p^3}{M^2} + \frac{kx^2 p}{M} \right\} - \frac{\hbar^2 k}{4M} \partial_p^2 p \right) + \left\{ \frac{p}{M} \right\} \right] W(x, p, t) \quad (15)$$

$$\text{and} \quad J_p = \left[ \Lambda^2 \left( \frac{\hbar^2 k^2 x}{4} \partial_p^2 - \left\{ k^2 x^3 + \frac{kxp^2}{M} \right\} + \frac{\hbar^2 k}{4M} \partial_x^2 x \right) - \{kx\} \right] W(x, p, t), \quad (16)$$

where the curly brackets surround the classical terms. All other terms (of order  $\mathcal{O}(\hbar^2)$ ) are of quantum origin.

For symmetry reasons the quantum terms cancel for eigenstates but not otherwise and are responsible for the non-Liouvillian nature of quantum phase space flow of superposition states of the Kerr oscillator. For energy eigenstates, Eq. (12) reads

$$\nabla \bullet \mathbf{w} = -\frac{\mathbf{J} \bullet \nabla W}{W^2}. \quad (17)$$

For eigenstates of the Kerr system,  $\mathbf{J}$  is always perpendicular to  $\nabla W$  and therefore quantum phase space flow is Liouvillian for its eigenstates.

For a superposition state (depicted in Fig. 2) Wigner flow is non-Liouvillian and forms isolated flow stagnation points at the intersections of the lines of vanishing  $J_x$ -component of the flow (thick green lines in Fig. 2) with lines of vanishing  $J_p$ -component of the flow (thick blue lines in Fig. 2). The flow's corresponding stagnation points are depicted by red plus-signs, if their Poincaré index  $\omega = 1$ , and by yellow minus signs, if their Poincaré index  $\omega = -1$ .

## V. WIGNER FLOW OF ANHARMONIC OSCILLATORS

For Hamiltonians of the form (6) with an anharmonic potential  $U$  it is no longer true that the divergence of  $\mathbf{w}$  for eigenstates is zero. In this case Wigner flow typically expands or compresses, i.e., is non-Liouvillian always, almost everywhere in phase space. This can be understood from the previous discussion of Eq. (9). The quantum terms in Wigner flow yield terms that break the incompressibility of classical phase space flow [6] and there are no symmetries, such as those for the eigenstates of the Kerr system, to offset their influence.

For illustration we show the Wigner flow portrait and the associated divergence map for the first excited bound state of a Morse oscillator in Fig. 3.

In the case of mechanical quantum systems, described by Hamiltonians of the form (6), the (black dashed) line of zero of the Wigner function, according to Eq. (9), coincides with (thick green) lines of zero of the  $J_x$ -component. According to Eq. (12) this is the location where the divergence of the Wigner phase space velocity  $\mathbf{w}$  becomes unbounded. The (thick blue) lines of vanishing  $J_p$ -component of the flow do typically not coincide with  $J_x$ -zero lines; this leads to the formation of isolated stagnation points of the flow [5, 12] wherever (off the  $x$ -axis) blue and green lines cross each other, see Fig. 3. In other



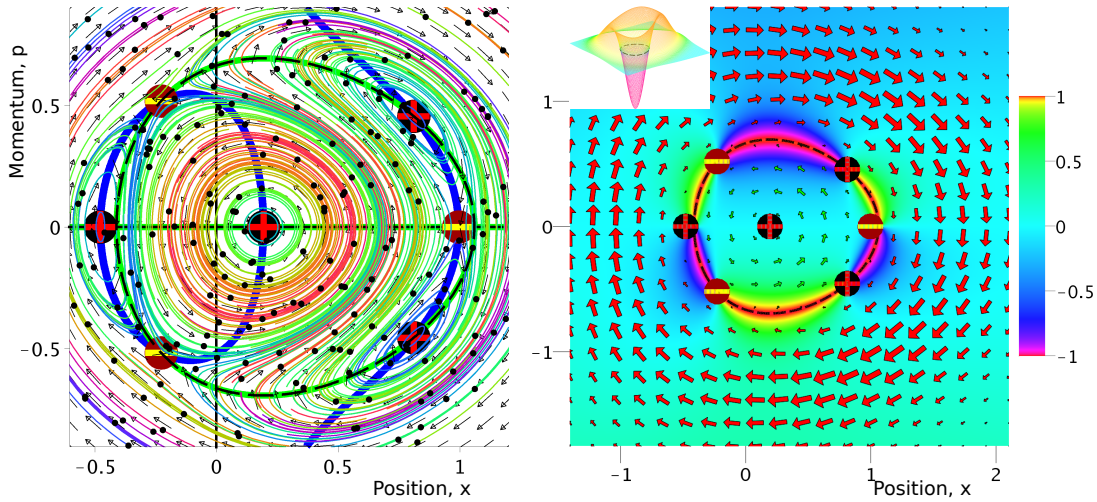


FIG. 3. (Color online) First excited energy eigenstate of the Morse oscillator with potential  $U(x) = 8(1 - \exp[-\frac{x}{4}])^2$  ( $M = 1$  and  $\hbar = 1$ ). Left: Streamlines of Wigner flow  $\mathbf{J}$  and its stagnation points (as in Figs. 1 and 2). Right:  $\frac{2}{\pi} \arctan(\nabla \bullet \mathbf{w})$  with  $\mathbf{J}$  superimposed (Wigner function shown in inset;  $\mathbf{J}$ -vectors are colored red for  $W > 0$  and green if the flow is inverted because  $W < 0$ ). For an anharmonic oscillator (6) Wigner flow is non-Liouvillian ( $\nabla \bullet \mathbf{w} \neq 0$ ) always, almost everywhere.

words, when we follow the line of unbounded divergence of  $\mathbf{w}$  we trace out the line where  $J_x = 0$ . If such a line crosses (off the  $x$ -axis) with a line where  $J_p = 0$ ,  $\nabla \bullet \mathbf{w}$  changes sign, this leads to the formation of the pinch-points of  $\nabla \bullet \mathbf{w}$  evident in the right panel of Fig. 3. Off the  $x$ -axis, these pinch-points thus coincide with flow stagnation points.

## VI. CONCLUSION

We introduce the concept of the Wigner phase space velocity  $\mathbf{w}$ . We show that the quantum-Liouville equa-

tion (4) is generically non-Liouvillian and would better be called quantum-continuity equation. Only in the case of the harmonic oscillator is the flow of the Wigner phase velocity divergence-free. Generically, for any anharmonic quantum-mechanical oscillator, Wigner flow is non-Liouvillian and features unbounded divergence. Field-oscillators of the Kerr type show intermediate behaviour in that their eigenstates feature Liouvillian flow, but their coherent superpositions do not. In anharmonic quantum-mechanical systems (6) the (off-axis) pinch-points of unbounded divergence of Wigner's phase space velocity  $\mathbf{w}$  coincide with the stagnation points of Wigner flow  $\mathbf{J}$ .

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